



Turning Concepts  
into Reality

# **The Analysis Enterprise**

## ***Tools for High Consequence Simulation***

***Advanced Simulation: A Critical Tool for Future Nuclear Fuel Cycles  
A National Laboratory Workshop***

**December 14-16, 2005**



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**Leader, Methods Development Group**  
**Lead, W Program ASC Advanced Applications**

Work performed under the auspices of the U.S. Department of Energy by the University of California,  
Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

# The Methods Development Group



- MDG was organized in the 1970's to create, maintain and continuously improve a set of tools for large-scale engineering simulation at LLNL
- Primary focus on nonlinear solid mechanics incorporating
  - Large deformation continua and structural elements
  - Finite strain constitutive models
    - E.g., metals, foams, rubbers, composites, geomaterials
  - Contact/impact
  - Heat conduction
- MDG's principal software products
  - DYNA3D/ParaDyn - explicit time integration for high-frequency structural dynamics
  - NIKE3D - implicit time integration for quasi-statics and low-frequency response
  - TOAPZ3D - implicit time integration for heat transfer
  - Diablo - parallel, implicit multi-physics
- MDG works closely with LLNL programs
  - Over 100 people in multiple directorates have access to the software

**Software plus skilled analysts with developer consultations produce the simulation product**

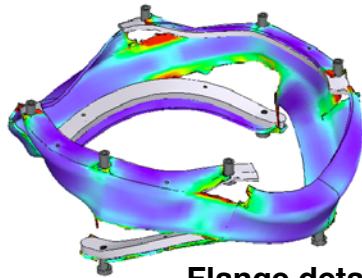
**The Analysis Enterprise**



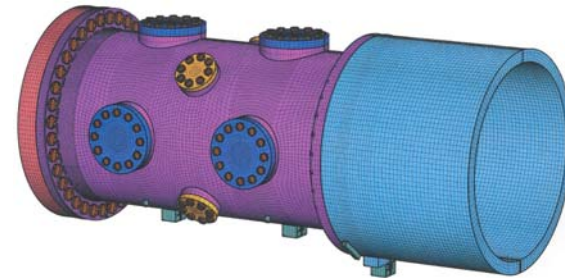
# ParaDyn provides nonlinear structural dynamics capabilities on ASC platforms



- In CY04, ParaDyn used for two million CPU-hours of throughput on LLNL parallel platforms
- Used daily for engineering analysis and decisions

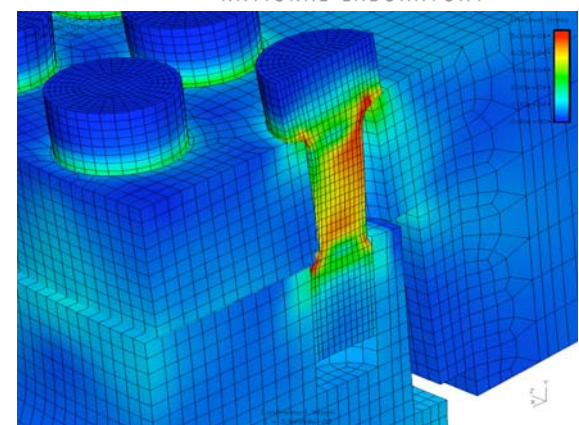
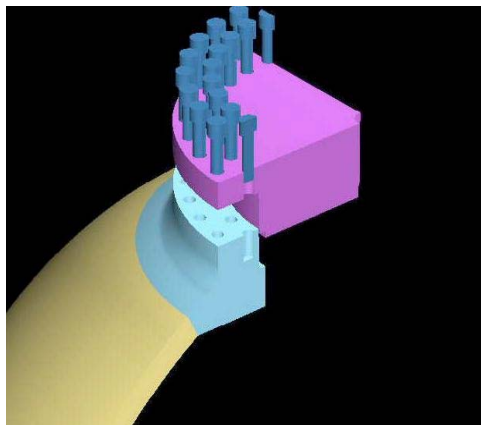


Flange detail from a transportation container courtesy Dan Badders



Sub-critical containment courtesy Kevin Roe

- A major engineering workhorse at Los Alamos, too.



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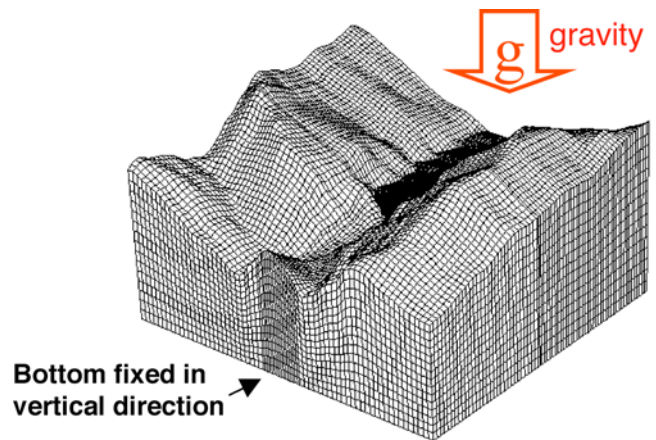
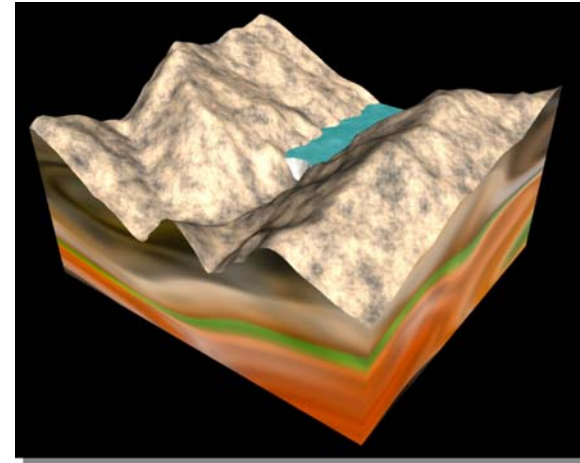
Hydrodynamic containment vessel courtesy LANL Engineering Sciences & Applications

# MDG tools applied to infrastructure assessments performed here...

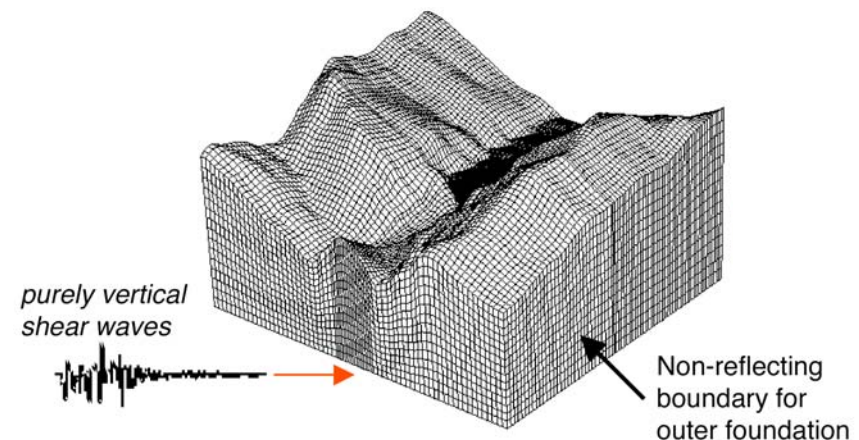


## • Work for Bureau of Reclamation

- Analyst-led effort (Noble, McCallen, *et al.*)
- Effects of local topography and rock jointing included in assessment of seismic response
- Illustrates need for complementary implicit and explicit FEM response calculations
- Simulation methodology migrated to BuRec



NIKE3D Static Initialization with  
Zero Displacement Control B.C.'s



DYNA3D Seismic Analysis





# MDG tools applied to infrastructure assessments performed here and elsewhere

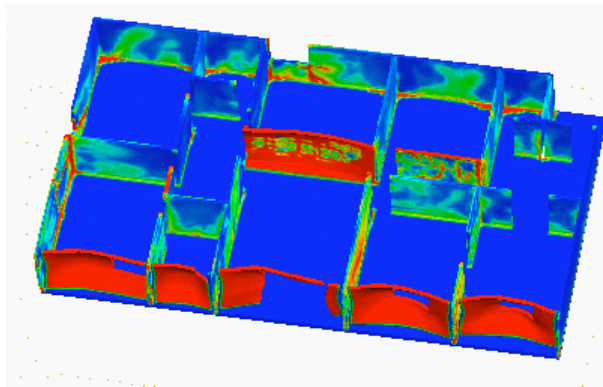
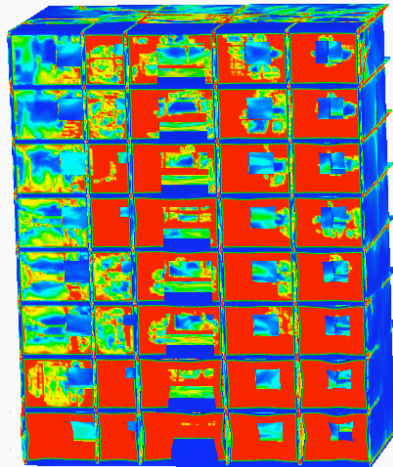


- US Army Engineer R&D Center

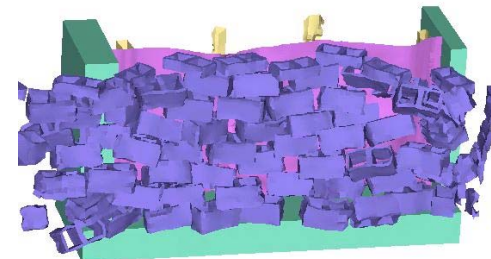
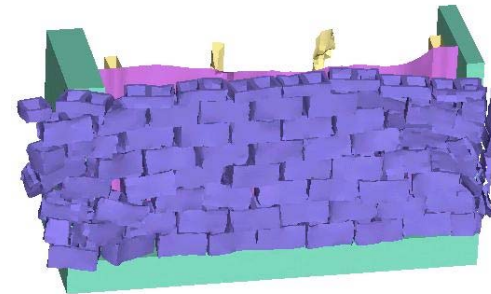
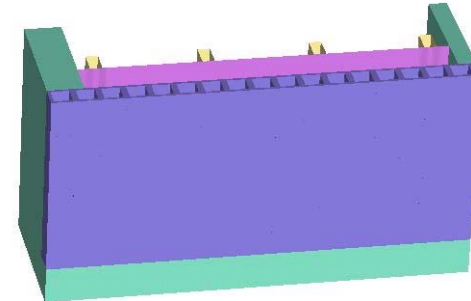


USAE ERDC

Apartment model with  
30 million DOFS  
courtesy P. Papados



Coupled CTH/ParaDyn blast structure simulation



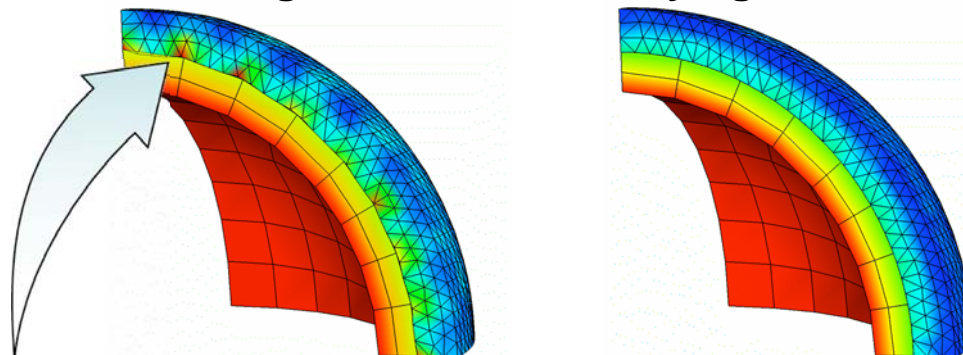
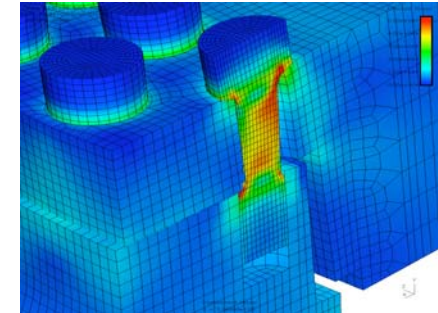
Building retro-design with textile liner



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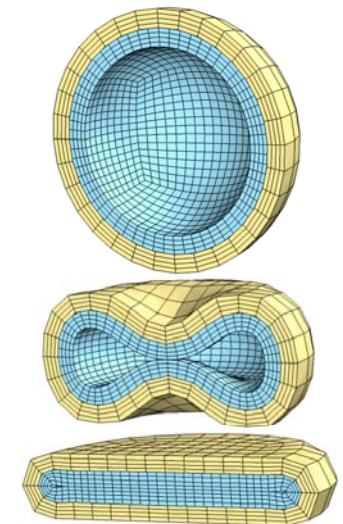
# Contact Methods a focus both for parallel implementations and fundamental formulations

- Unbonded material interfaces have strong effects on many mechanical and structural assemblies →
- Mortar Methods achieve mathematical consistency through segment-on-segment projections & constraints
  - Retain convergence of the underlying FEM



- Mortar methods eliminate singularities from typical node-on-segment methods

- This work extended academic efforts for 2D linear problems to 3D curved surfaces on irregular meshes & finite deformations
- Research now being “hardened” by practical application to programmatic needs

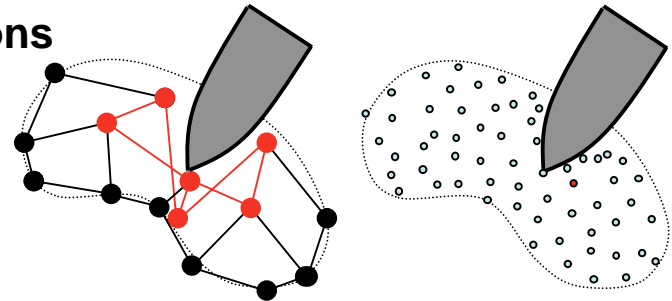


# Several current LDRD projects contribute to ongoing enhancements of MDG's capabilities



- **Natural Element Method (Puso & Zywicz)**

- “Mesh-less” to accommodate extreme deformations
- Penetration without pre-seeded perforation
- Still Lagrangian for material model

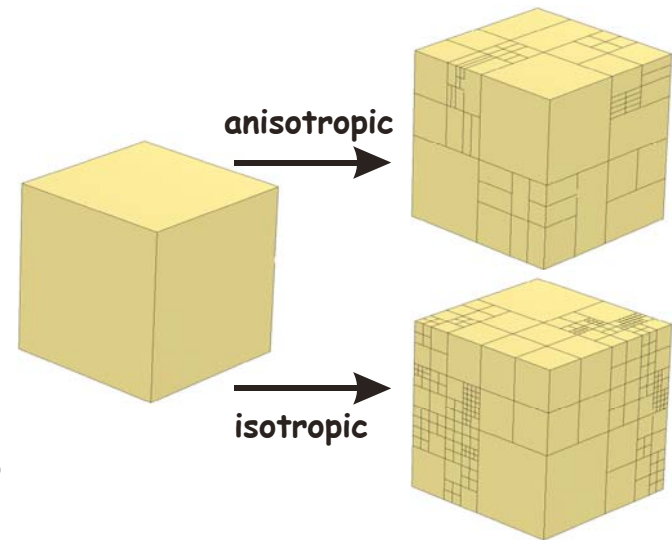


- **Electro-thermo-mechanical (combined EE & ME)**

- Advanced, higher-order EM capabilities being interfaced to multiple thermo-mechanics codes: Diablo and ALE3D

- **Adaptive Mesh Refinement (Parsons & Solberg)**

- Provide feedback on quality of solution and automatically drive toward a better mesh
- Research robust error estimators for nonlinear solid mechanics problems of interest to LLNL
- Unique capability for anisotropic refinement
- Requires lots of infrastructure – this was the time to get in on the the ground floor of the Diablo architecture

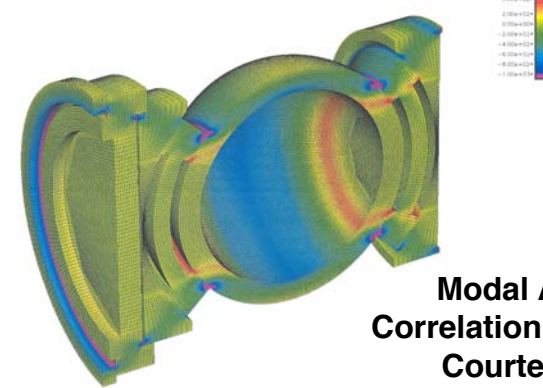
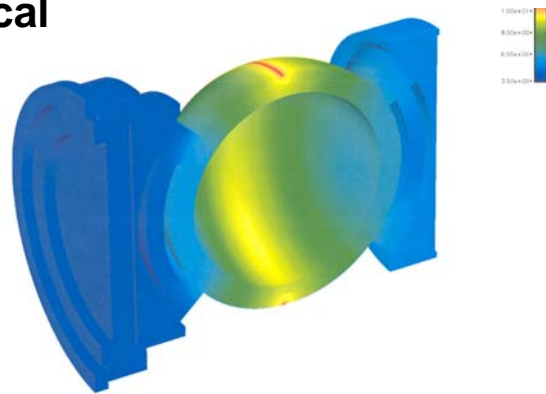


# The Diablo code project is building an implicit capability to complement ParaDyn



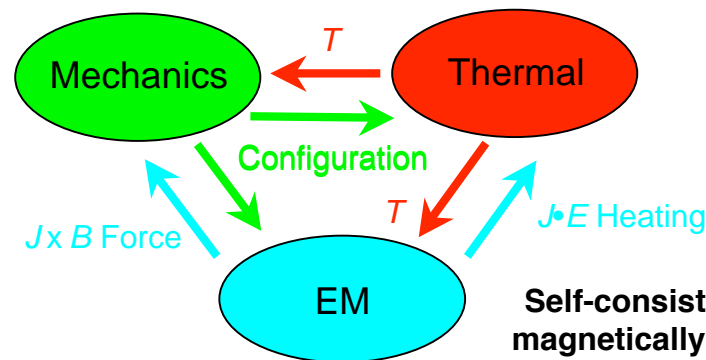
- Migrating nonlinear capabilities of NIKE3D & TOPAZ3D to ASC platforms
- Creating a software architecture for multi-field problems, e.g.,
  - Thermo-mechanical

Thermal and stress response to heat flux at waist of assembly



Modal Analysis  
Correlation Experiment,  
Courtesy AWE

- Thermo-chemical for surface corrosion (eventually coupled with mechanics)
- Electro-thermo-mechanical
- Creating links to third-party CFD



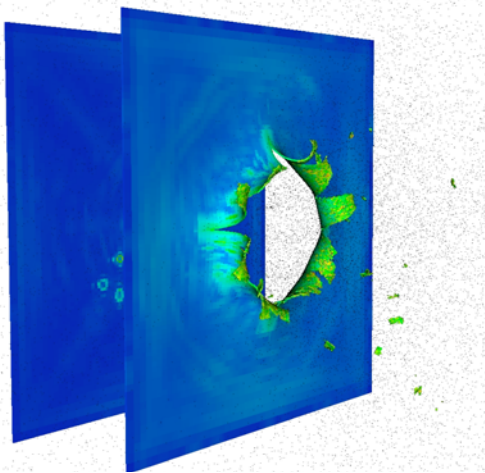
Self-consistent coupling for  
magnetically driven materials



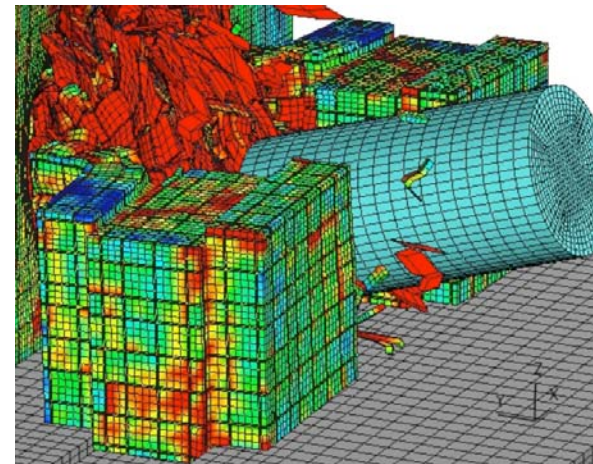


# MDG codes leverages material model developments both internal and external

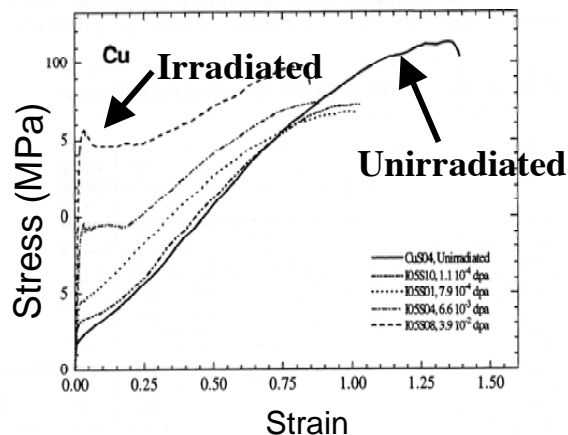
- Steinberg-Guinan with 3D failure (W. Moss, LLNL)



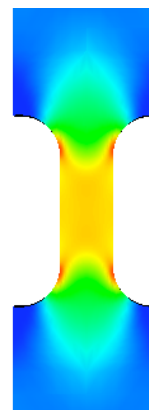
- DTRA Concrete Model (Malvar *et al.*, Karagozian & Case) courtesy Ed Kokko



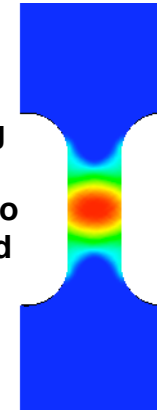
- We can leverage LLNL's investment in multi-scale modeling and specialized models such as radiation damage by Arsenlis & Wirth



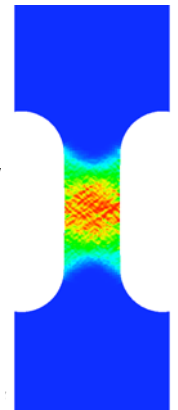
Ferencz-1;  
UCRL



Low hardening  
of irradiated  
material leads to  
localization and  
less ductility



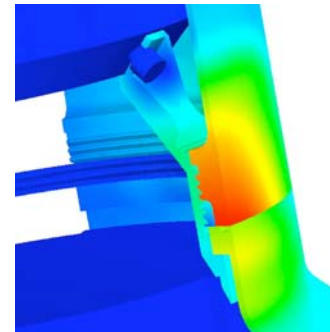
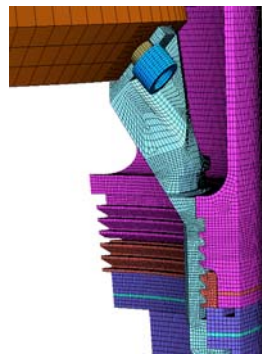
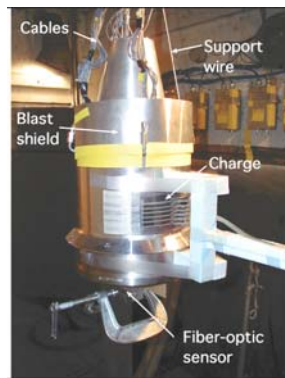
Role of spatial  
inhomogeneity  
can also be  
assessed



# ASC is building engineering simulation tools for high consequence analysis



- The role of Verification & Validation is substantial
  - MDG tools benefit from independent validation, e.g.,  
LANL multi-year study of a complex threaded joint under impulse load



**Los Alamos**  
NATIONAL LABORATORY  
Doebeling *et al.*,  
LANL ESA-WR

- Will need to “harvest” applicable past experiments and plan new ones
- MDG tools and experienced LLNL analysts can contribute engineering insight and decision making to new technology and design efforts
- MDG can partner with outside expertise, e.g., material models and other simulation capabilities, and support migration to other participants





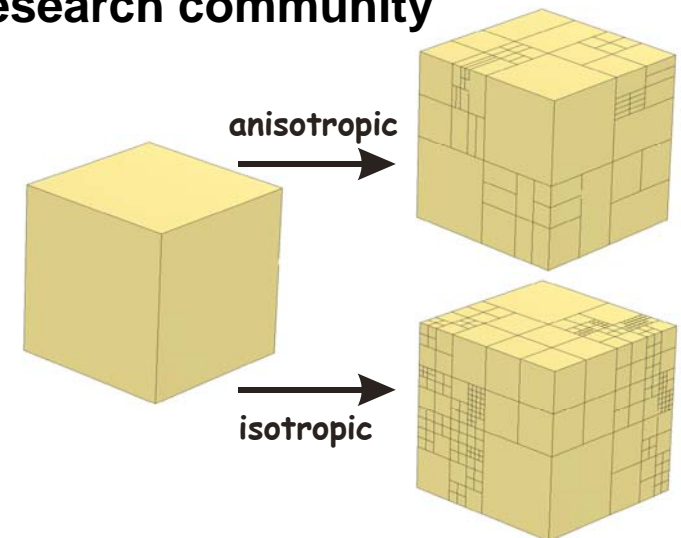
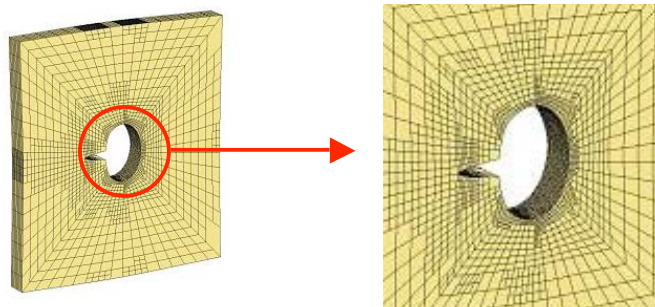
## ***BACKUP SLIDES***



# Adaptive Mesh Refinement is a technology being made applicable to our problems



- When is a mesh good enough? AMR gives quantitative feedback.
- Relevant issues
  - Unstructured meshes for engineering geometries
  - Large-scale parallel implementation for ASC class computers
  - Robustness of error estimators for real-world nonlinear solid mechanics
- The first two issues required significant up-front programming investment
- The third issue will be our contribution to the research community
- Highlights to date:
  - Anisotropic refinement is a unique capability
  - Refinement to curved boundaries

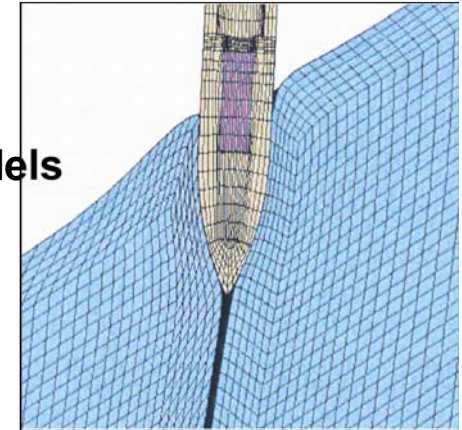
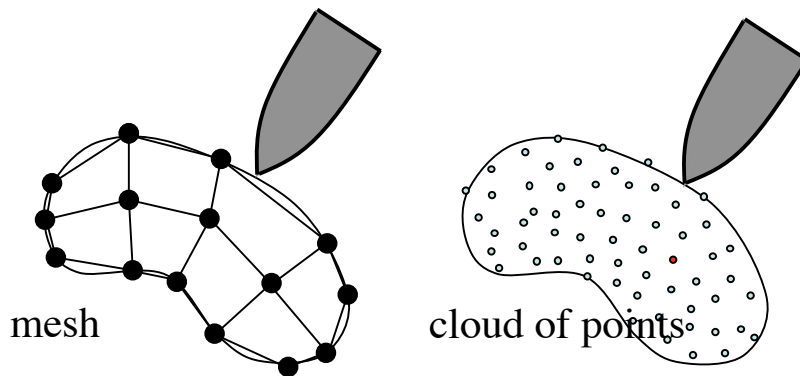




# Natural Element Methods for Extreme Deformation



- Penetration and other problems break down Lagrangian FEM
  - Need to model beyond local material failure
- Developing new “mesh-less” methods
  - Keep Lagrangian description for compatibility w/ material models



Historical approach  
with pilot hole

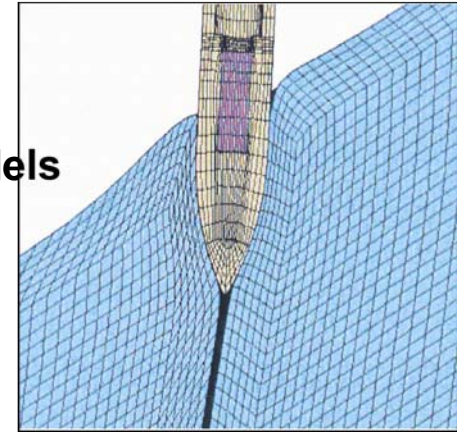
- Key idea: adaptive integration using Voronoi Diagram
- Early results promising - First paper already in submittal
- Project providing foundation for collaboration with J.S. Chen of UCLA
- This technology *alone* will not solve penetration modeling needs
  - E.g., need target material modeling and characterization



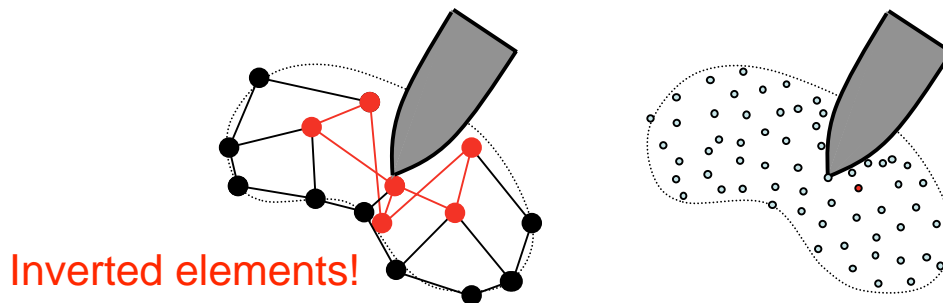
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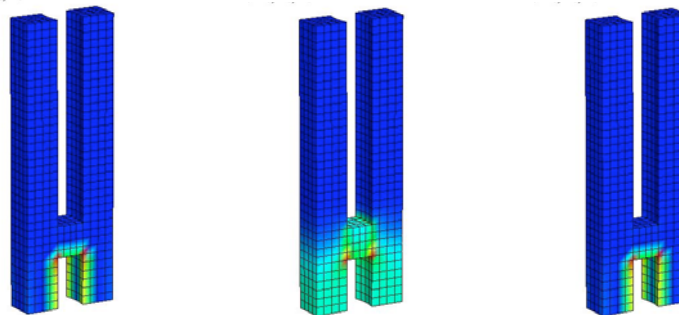
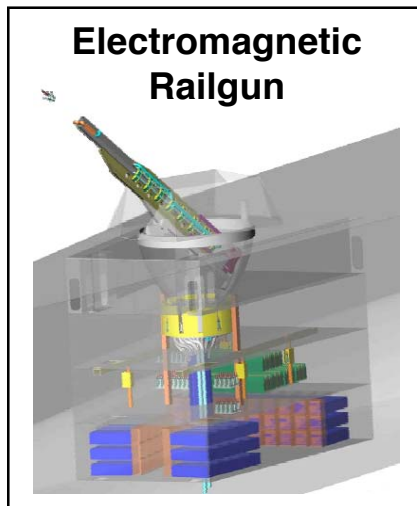
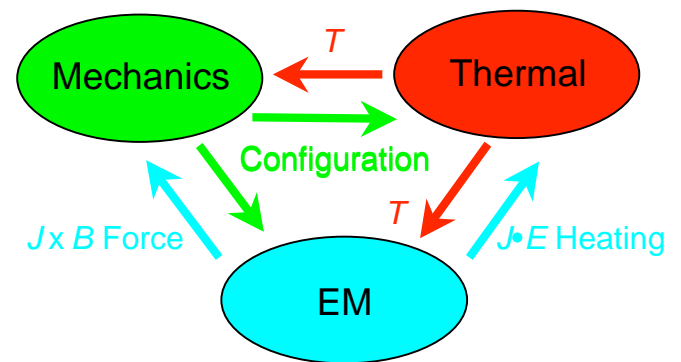
Inverted elements!

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# Electro-Thermo-Mechanical Coupling

- Historically, we had little experience dealing with systems where the electromagnetic and thermo-mechanical response share time scales
  - “Hand it over the wall and leave me alone” coupling was good enough
- Magnetically Driven Materials initiative requires capabilities for solving ETM simultaneously in a self-consistent manner
  - EM being made available to multiple thermo-mechanics codes: Diablo and ALE3D



- Force / Current / Heating on *notional* railgun  
(Bounding air domain removed; static configuration)